Complex Fluids in Manufacturing

Workshop - 21 April 2021

CORAL project dissemination initiative

Book of Abstracts

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The British Society of Rheology

FACULTY OF MATHEMATICAL AND PHYSICAL SCIENCES
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Workshop Programme

09:30 – Welcome

9:45 – Geoff Maitland (Imperial College London)
"*Formulation challenges for some oilfield complex fluids* "

10:15 – CORAL project overview (presented by Giota Angeli, UCL)
"*Manufacturing Challenges of Viscoelastic Suspensions*"

BREAK

11:00 – **Short presentations**

Pavlos Stefanou (Cyprus University of Technology): "*Coupling theory and simulations to fully elucidate the important role of end groups in poly(ethylene glycol) - silica nanocomposite melts*"

Soichiro Makino (University of Edinburgh): "*Rheology of granular-gel composite suspensions*

11:30 – Serafim Bakalis (University of Copenhagen)
"*Product Engineering: Can we move away from trial and error approaches?*"

BREAK

13:00 – Yiannis Dimakopoulos (University of Patras)
"*Advanced Computational Methods for the Simulation of Complex Fluids in Industrial Processes*"

13:30 – **Short presentations**

Jurriaan Gillissen (UCL): "*Modelling the Microstructure and Stress in Dense Suspensions under Inhomogeneous Flow*“

Andreia F. Silva (ECFP/University of Edinburgh): "*Rheological design of thickened alcohol-based hand rubs*“

Liam Escott (UCL): "*Modelling a suspension of slightly deformable particles in a weakly viscoelastic fluid*"

14:00 – Sophie Darragh (GSK)
“*Challenges in Industrial Processing of Complex Fluids*”

BREAK

14:45 – Randy Ewoldt (University of Illinois at Urbana-Champaign)
"*Designing complex fluids for flow objectives*"

15:15 – Suzanne Fielding (Durham University)
"*Ductile and brittle yielding in sheared amorphous materials*"

About the CORAL Project

CORAL project Overview: *Manufacturing challenges of viscoelastic suspensions*

presented by **Panagiota Angeli**
Department of Chemical Engineering, University College London (UK)

The CORAL (Complex ORAL health products) project, funded by the EPSRC Future Formulations programme, sought to introduce new fundamental insights into complex formulations and address related manufacturing challenges. Within this project, thanks to the multi-disciplinary expertise of the researchers involved, we were able to implement cutting-edge experimental techniques to characterize complex fluids- including viscoelastic fluids and suspensions of particles- over multiple scales; to derive constitutive equations that describe their rheological behaviour using advanced mathematical modelling; and to develop a Computational Fluid Dynamics (CFD) framework for predicting their fluid dynamic behaviour, validating our results against advanced experiments on model systems. With a direct sight on translation, the project also addressed the process scale-up challenges and the issues of manufacturability in current batch processes, proposing innovative solutions to enable new continuous-flow intensified technologies. Our exemplar focus on non-aqueous oral care formulations offered solutions that directly impact the manufacturing of novel formulations in the pharmaceutical, food and cosmetics industries as well as the development of inkjet printing and additive manufacturing technologies.

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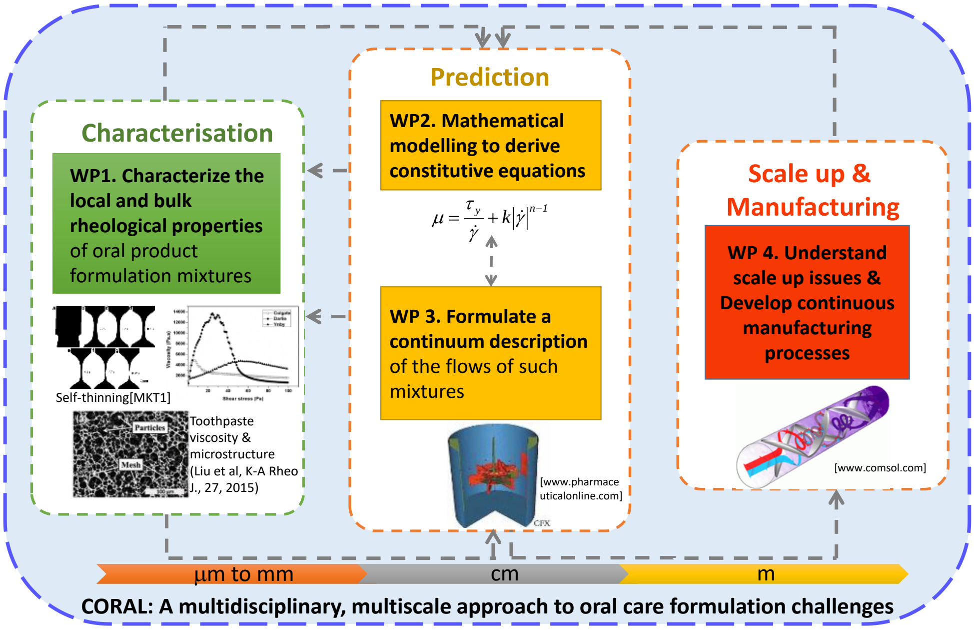

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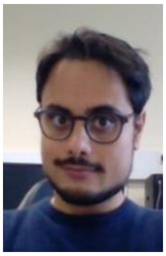

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Keynote Speakers

Formulation challenges for some oilfield complex fluids

Geoff Maitland

Department of Chemical Engineering, Imperial College London (UK)

The talk will centre on the formulation complex fluids used in the construction of oil and gas wells and in the optimisation of the hydrocarbon recovery process. It will start with a brief overview of these processes and the functional properties required of these fluids, explaining why the fluid properties sometimes need to be modified during the process, requiring real-time formulation. Some observations will be made on how the combination of experiments, theory and fluid simulation is increasingly transforming fluid formulation from an empirical art into a more robust engineering process. This approach will be illustrated with a number of case studies of the formulation of smart complex fluids for a range of oilfield operations which all require careful control of fluid rheology and its variation with well/reservoir conditions, including Hydraulic Fracturing, Water Control, Well Drilling, Shale Swelling and Sand Consolidation.

About the Speaker

Geoff Maitland is Professor of Energy Engineering at Imperial College London since 2005 and a Past President of the Institution of Chemical Engineers (2014-15). His career has spanned academia and industry, spending 20 years in oil and gas with Schlumberger and over 20 years at Imperial. He studied Chemistry at Oxford University where he also obtained his doctorate in Physical Chemistry. After a period as an ICI Research Fellow at Bristol University, he was appointed to a lectureship in Chemical Engineering at Imperial College in 1974. His research focused on molecular interactions and the transport properties of fluids, including polymer systems. He held a number of senior technical and research management positions in Cambridge and Paris, most recently as a Research Director. His current research is centred on how we can continue to use fossil fuels for most of this century without causing catastrophic climate change, particularly through carbon capture and storage (CCUS).

He has chaired several CCUS public reports and been a member of the 2018 UK Government CCUS Cost Challenge Taskforce. Geoff is a Fellow of the Institution of Chemical Engineers, the Royal Society of Chemistry and the Energy Institute. He was awarded the Hutchison Medal by the Institution of Chemical Engineers in 1998 and served as President of the British Society of Rheology from 2002-2005. In 2017 he was awarded the Leverhulme Medal of the Society of Chemical Industry. He is the Founding Director of the Qatar Carbonates and Carbon Storage Research Centre, a $70M 10 year academic-industry research programme based at Imperial College London, and is currently Director of the Shell-Imperial Digital Rocks Lab. He was appointed CBE in 2019 for services to Chemical Engineering.

Product Engineering: Can we move away from trial and error approaches?

Serafim Bakalis

Department of Food Science, University of Copenhagen (DK)

The increasing need to develop new sustainable diets has increased the need to develop new ways that we design foods. It is of special interest to design foods through an Understanding of digestion and absorption of nutrients and to develop models that could be able to predict the food behavior thought the gastrointestinal tract. In order to achieve this, we have build a range of tools including an in vitro small intestine model (SIM) that was used to build starch digestion and glucose absorption as function of food viscosity. The effect of mixing and food formulation was evaluated and correlated to changes on glucose absorption. Finite element analysis was used to understand the effect of segmentation on nutrients absorption as well as bolus break up. Overall, this combined methodology could provide a transformation of the ways that formulated products are designed.

About the Speaker

Prof. Serafim Bakalis has obtained a BS in Chemical Engineering form National Technical University of Athens, Greece and a PhD in Food Science. He is currently a Professor in Dairy product technology in the Department of Food Science in University of Copenhagen. His interests are in investigating transport phenomena using a range of experimental and numerical techniques. His skills are applied to understand performance and design Sustainable and Healthy Products.

Advanced Computational Methods for the Simulation of Complex Fluids in Industrial Processes

Yannis Dimakopoulos

Chemical Engineering, University of Patras (GR)

Simulation of the flow or the deformation of industrial materials exhibiting viscoelastic or viscoplastic behavior has always been challenging. The origins of the numerical difficulties are associated with the structure of the material and its modeling approximation. In the case of viscoplastic material, e.g., dense suspensions, the discontinuity at the yielded-unyielded interface requires special handling [1]. For this purpose, a modification of the Augmented Lagrangian (AL) method has recently been proposed, namely, the Penalized Augmented Lagrangian method [2], which exhibits shorter computation times and the same accuracy compared to the existing AL methods. On the other side, a new finite element formulation for viscoelastic flows [3, 4] has been proposed by our group that uses equal order of interpolants for all variables along with the conventional finite element stabilization techniques, like the PSPG. We couple the PAL algorithm with the new finite element formulation to present an even faster and stabler method for the computation of viscoplastic flows, the so-called PAL-PSPG technique. The efficiency of the new framework is testified by comparing the numerical results of our method to those of the literature. We perform mesh-convergence tests illustrating that both the PAL and the PAL-PSPG feature an almost 1st order accuracy in space. The mesh-convergence order is limited by the PAL method itself and not from the low-order interpolants of variables, making the new formulation even more attractive.

[1] E. Mitsoulis, J. Tsamopoulos, Rheol. Acta 56 (2017): 231-258.
[2] Y. Dimakopoulos, G. Makrigiorgos, G.C. Georgiou, J. Tsamopoulos, J. Non-Newtonian Fluid Mech 256 (2018): 23-41.
[3] S. Varchanis, A. Syrakos, Y. Dimakopoulos, J. Tsamopoulos, J. Non-Newtonian Fluid Mech 267 (2019): 78-97.
[4] S Varchanis, A Syrakos, Y Dimakopoulos, J Tsamopoulos, Journal of Non-Newtonian Fluid Mech 284 (2020), 104365.

About the Speaker

Dr. Yannis Dimakopoulos is an Associate Professor. He received the Master's and Ph.D. degrees from the Chemical Engineering Department of the University of Patras in 2003. In 2005 & 2006, he was a post-doctoral associate of the Laboratory of Computational Fluid Dynamics. In 2007, he joined the Biomedical Engineering and Soft Tissue Engineering group of the Biomedical Engineering Department of the Eindhoven Technological University in the Netherlands. From 2011 to 2013, he was an adjunct Lecturer at Chemical Engineering Department at UPatras. From 2012 to 2014, he worked as a researcher for the University of Cyprus. In January 2014, he was appointed as Assistant Professor, and in September 2019, he was promoted to Associate Professor. His research and teaching works are related to Fluid Mechanics, Computational Rheology of Complex Fluids, Computational Transport Phenomena, Advanced Numerical Methods, and Large-Scale Computational Techniques with applications in the study of synthetic and biological fluid flows.

Among the distinctions in his career, the Walter Prize for the best 2018 publication in the Journal of Non-Newtonian Fluid Mechanics stands out.

Challenges in Industrial Processing of Complex Fluids

Sophie Darragh

GlaxoSmithKline Consumer Healthcare (UK)

GSK Consumer Healthcare develop a wide range of Oral Healthcare products. These products must meet various demands; they must be stable, effective and appealing to the end-consumer. In order to meet these requirements, these product contain a wide range of varying components. The combination of these components results in complex Non-Newtonian fluids with multiple interfaces (solid-solid, solid-liquid, liquid-liquid, liquid-air and solid-air!) which are exceedingly challenging to understand and manufacture. The talk will focus on some of the current challenges faced during manufacture of complex semi-solids and how these are being currently explored and managed.

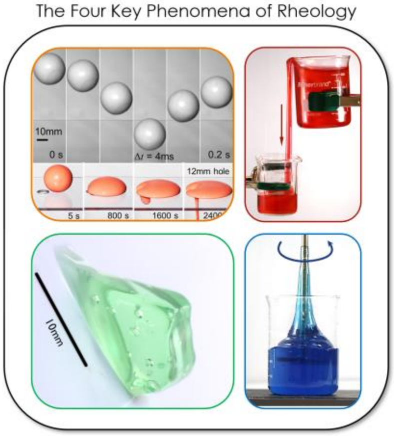
About the Speaker

Sophie is a Principal Process Engineer at GSK Consumer Healthcare R&D based in Weybridge, Surrey with an academic background in Colloid Chemistry – particularly the behaviour of solid particles at fluid interfaces. Sophie has extensive knowledge and experience on industrial processing of Emulsions and Semi-Solids for GSK Pharma and Consumer Healthcare products in addition to their characterisation (with a focus on Rheology of complex semi-solids).

Designing complex fluids for flow objectives

Randy H. Ewoldt
Mechanical Science and Engineering, University of Illinois at Urbana-Champaign (USA)

A small step away from Newtonian fluid behavior creates an explosion in the range of possibilities. Non-Newtonian fluids can achieve diverse design objectives, but the complexity introduces challenges. From a design perspective, this talk will review successes and methods in answering: How can non-Newtonian properties help? What properties are optimal? How can we get those properties? Design methods are illustrated with examples: linear viscoelasticity for vibration isolation, nonlinear viscoelasticity for tribological friction reduction, extensible yield-stress fluids for direct-write 3D printing inks, and yield-stress fluid design for wildland fire suppression (and splashy art).



About the Speaker

Randy H. Ewoldt is an Associate Professor in the Department of Mechanical Science and Engineering at the University of Illinois at Urbana-Champaign (UIUC). Dr. Ewoldt received his Ph.D. (2009) and M.S. (2006) from MIT, and B.S. (2004) from Iowa State University. Before joining UIUC, he was a postdoc at the University of Minnesota. He conducts fundamental research in fluid mechanics and rheology. This includes new measurement methods and paradigms for design with materials such as yield-stress fluids, polymer gels, and biological materials. Dr. Ewoldt is a recipient of a 2014 NSF CAREER Award, the 2014 Arthur B. Metzner Early Career Award from The Society of Rheology, a 2017 Presidential Early Career Award for Science and Engineering (PECASE), and awards from ASME, 3M, DuPont, and TA Instruments. His teaching has been recognized by awards from his department, college, and alumni of UIUC. He regularly lectures at rheology short courses in the USA and Europe. In 2018 he was a Guest Professor at ETH-Zürich, Switzerland, in the Department of Materials.

Ductile and brittle yielding in sheared amorphous materials

Suzanne Fielding
Department of Physics, Durham University (UK)

We review recent progress in understanding the nature of yielding in amorphous materials. Within an athermal elastoplastic model in quasistatic shear, we find that yielding is brittle in the limit of large system size, whatever the level of annealing/ageing of the sample prior to shear. For small systems, in contrast, we find a crossover from apparently ductile to brittle yielding behaviour with increasing degree of sample annealing prior to shear. Time permitting, we will also make some remarks about the difference between the nature of ductile/brittle yielding in thermal vs athermal materials.

About the Speaker

Suzanne Fielding obtained her first degree in Physics from Oxford University in 1997 and her PhD from Edinburgh University in 2000. Following postdoctoral research at Leeds University, she spent four years lecturing in applied mathematics at Manchester University, before moving to the Department of Physics at Durham University in 2009. In 2010, she received the Arthur B. Metzner award of the Society of Rheology. Financial support for her research has been provided by an EPSRC Postdoctoral Research Fellowship in Theoretical Physics, an EPSRC Advanced Research Fellowship, the EPSRC funded SOFI-CDT, industrial companies such as Schlumberger Cambridge Research Ltd, and most recently with a European Research Council Advanced Grant, which started in 2020. Her research interests lie in the theoretical and computational statistical mechanics and rheology (deformation and flow properties) of soft materials and complex fluids such as colloids, emulsions, foams, microgels, surfactants, liquid crystals, and polymers, and their biological counterparts such as bioactive fluids and biological tissues.

Short Presentations

Coupling theory and simulations to fully elucidate the important role of end groups in poly(ethylene glycol) - silica nanocomposite melts

Pavlos Stefanou

Department of Chemical Engineering, Cyprus University of Technology (GR)

Polymer nanocomposites comprise a class of nanostructured materials where nano-sized particles are embedded in a host polymer matrix in order to improve its properties (mechanical, transport, electrical, etc.). In the present work, we combine molecular dynamics (MD) simulations and Rouse theory suitably adapted for polymer chains adsorbed by one or both of their ends to offer a quantitative description of local structure and microscopic dynamics in attractive polymer nanocomposite melts using as a model system a poly(ethylene glycol) (PEG)-silica nanocomposites. Our work reveals that adsorbed polymer segments in the form of tails and loops on silica exhibit appreciable mobility locally. The simulations also reveal that PEG chains terminated with hydroxyl groups are primarily adsorbed on the silica surface by their ends giving rise to a brush-like structure, whereas PEG chains terminated with methoxy groups are adsorbed equally probably along their entire contour. Direct comparison of simulation and theoretical predictions, in which information from the MD simulations are used as input, with previously reported experimental data in the literature for the dynamic structure factor for the same systems under the same temperature and pressure conditions reveals excellent agreement.

About the Speaker

Dr. Pavlos S. Stephanou graduated from the Department of Chemical Engineering, University of Patras (Greece) in 2006. He then pursued postgraduate studies at the same department under the guidance of Prof. Vlasis Mavrantzas. His PhD thesis is entitled “Development of scale-bridging methodologies and algorithms founded on the outcome of detailed atomistic simulations for the reliable prediction of the viscoelastic properties of polymer melts”. During his postgraduate career he has worked at the University of Cyprus (Cyprus), the ETH Zürich (Switzerland), the Cyprus University of Technology (Cyprus), and Novamechanics Ltd (Cyprus) having received numerous grants and awards. He received the «Cyprus Research Award – Young Researcher 2015» (Thematic area: Physical Sciences and Engineering) by the Research Promotion Foundation (RPF) of Cyprus, for his research work entitled «Modelling the viscoelasticity of polymer-based nanocomposites guided by principles of non-equilibrium thermodynamics». Since September 2019 he is an Assistant Professor at the Department of Chemical Engineering of the Cyprus University of Technology.

Rheology of granular-gel composite suspensions

Soichiro Makino
University of Edinburgh

Granular-gel composite suspensions composed of coexisting large repulsive and small attractive particles are encountered in a variety of industrial applications such as the manufacturing process of Lithium-ion battery cathodes. We investigate the rheology and microstructure of model composite suspensions where large non-functionalised silica particles are embedded in a colloidal gel formed by small attractive fumed silica particles. We find the state-transition behaviour which are reversible by pre-shear: solid-like state after high pre-shear and liquid-like state after low pre-shear. Cryo-SEM observation reveals that the small attractive particles are dispersed among the large repulsive particles under the high pre-shear, while these small particles form dense blobs under the low shear. These blobs have a core-shell structure, and also are condensed and reinforced by increasing the large repulsive particles. We summarise the rheological state in a state diagram and explore how the state boundaries on the diagram can be tuned by changing experimental parameters such as applied shear stress, volume fraction, and attraction strength. Finally, we propose key parameters to control the state-transition behaviour towards greater efficiency in Lithium-ion battery manufacturing.

About the Speaker

Soichiro Makino is a researcher at Toyota Central R & D labs., and also a PhD student at University of Edinburgh. After completing his master’s degree in mechanical engineering in 2008, he joined the company and has studied a wide range of manufacturing processes in car industry, such as chemical vapour deposition, heat treatment, and fibre moulding. In 2018, Soichiro started a new project related to suspension rheology in Lithium-ion battery manufacturing for electric vehicles. As a part of the project, he is currently studying the rheology of a model suspension for battery electrodes in PhD programme at University of Edinburgh, supervised by Prof. Wilson C. K. Poon and Dr. John R. Royer.

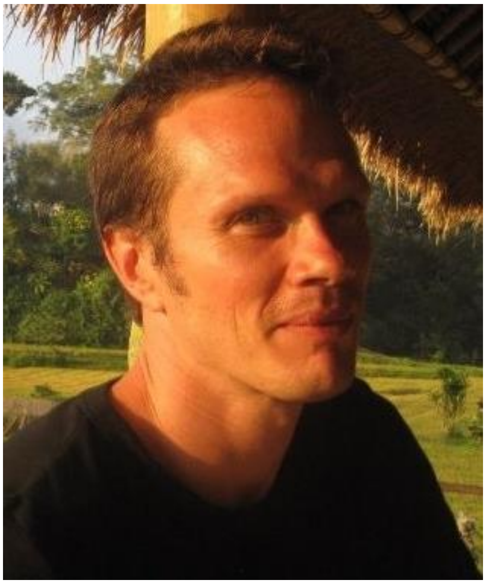
Modelling the Microstructure and Stress in Dense Suspensions under Inhomogeneous Flow

Jurriaan Gillissen
Department of Mathematics, University College London (UK)
The Technology Partnership, Melbourn (UK)

Under inhomogeneous flow, dense suspensions exhibit behaviour that violates the conventional homogeneous rheology. Specifically, one finds flowing regions with a macroscopic friction coefficient below the yielding criterion, and volume fraction above the jamming criterion. We demonstrate the underlying physics by incorporating shear rate fluctuations into a recently proposed tensor model for the microstructure and stress, and applying the model to an inhomogeneous flow problem. The model predictions agree qualitatively with particle-based simulations.

About the Speaker

Jurriaan obtained a PhD in computational fluid dynamics from Delft and after his PhD he worked for a decade in academia on fluid related problems.
Now Jurriaan works as a technology consultant at The Technology Partnership in Melbourn UK.



Rheological design of thickened alcohol-based hand rubs

Andreia F. Silva

Edinburgh Complex Fluids Partnership (ECFP), University of Edinburgh (UK)

The coronavirus 2019 (COVID-19) pandemic created an unprecedented demand for sanitising hand rubs that is expected to continue post-pandemic. The World Health Organization (WHO) has recommended alcohol-based hand rub (ABHR) formulations which contain 80% (v/v) ethanol or 75% (v/v) isopropyl alcohol as the active ingredient [1], however these formulations are low-viscosity Newtonian liquids making their pouring and rubbing on hands difficult due to rapid runoff. The rheological properties of ABHR are key to determine its 'hand feel' and 'rubbing capacity'. In this work we first propose several rheological design principles for thickened ABHRs, based on the concepts of runoff, spreadability, smoothness and non-stickiness. We then thicken the WHO formulation using different polymers (microgels and linear) and investigate if their rheological behaviour fits our proposed design principles. Results show that the WHO formulation thickened with microgels have a shear thinning and yield flow behaviour that fits most of our design principles. Linear polymers can also produce gels that have good spreadability, minimal runoff, and additionally offer a smooth feeling during rubbing due to the development of a finite first normal stress difference. The development of ABHRs that can offer a superior hand feeling is still an ongoing challenge.

About the Speaker

Andreia is a bioengineer with a PhD in complex fluids that has been using physical, chemical and mechanical techniques to understand both the macroscopic and microscopic behaviour of complex fluids and the contribution of isolated components with the aim of developing new formulations. Andreia is currently an Impact Acceleration Associate at The Edinburgh Complex Fluids Partnership (ECFP), The University of Edinburgh. She works in collaborative research projects with commercial partners, assisting industrial clients developing new products, technologies and materials in complex fluids/soft matter.

Modelling a suspension of slightly deformable particles in a weakly viscoelastic fluid

Liam Escott
Department of Mathematics, University College London (UK)

Suspensions of solid or fluid phases within a solvent medium has been a topic of interest for the rheological community, on both the experimental and theoretical side over the past century. Significant developments have been made in more recent years regarding the computational approach to a single sphere in non-Newtonian background fluid, notably in the range of small to medium effects of viscoelasticity. This is a step further than previous research in the area, which describes the contribution from deformed elastic solid to the bulk rheology using a Newtonian background fluid. This research includes the limitation that one must consider dilute volume fractions, determined by the volume ratio of solid to computational domain, and we attempt to address this by employing a cell model approach. This technique has the distinct advantage of being both simple and useable for industrial applications compared to the numerical simulations for similarly non-dilute solid volume fractions. We derive analytic solutions for viscometric functions of the suspension, using the second-order fluid model to describe the fluid domain, and a Hookean elastic model for the solid. Under the dilute limit, we show the agreement of our results with that of existing literature, along with a presentation of the contributions from hydrodynamic and deformation effects. Further, we show our predictions for the bulk rheology up to larger than dilute concentrations along with the relevant comparisons to experimental data.

About the Speaker

Liam is Masters graduate in Mathematics from University College London, with a specialisation in fluid dynamics. As a current PhD student at UCL, Liam is researching the application of analytical study in weakly viscoelastic systems to produce comparisons with computational and experimental data. Further, as of recently a short term Research Fellow position, focusing on the contribution and comparison to simulations in similar flows.

Acknowledgments

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Funders

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